Towards a Renormalization Group Approach to Density Functional Theory – General Formalism and Case Studies –

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We discuss a two-point particle irreducible (2PPI) approach to many-body physics which relies on a renormalization group (RG) flow equation for the associated effective action. In particular, the general structure and properties of this RG flow equation are analyzed in detail. Moreover, we discuss how our 2PPI RG approach relates to Density Functional Theory and argue that it can in principle be used to study ground-state properties of non-relativistic many-body systems from microscopic interactions, such as (heavy) nuclei. For illustration purposes, we use our formalism to compute the ground-state properties of two toy models.

I. INTRODUCTION

Originally, Density Functional Theory (DFT) has been invented by Hohenberg and Kohn to study atoms with many electrons in an efficient way [1, 2]. Since then, DFT has indeed been successfully used to study a large variety of quantum systems with many degrees of freedom, ranging from electronic systems over ultracold Fermi gases to (heavy) nuclei.

For heavy nuclei, DFT remains currently to be the only feasible approach for a calculation of ground-state properties [3]. In fact, the nuclear energy density functional approach represents a very active research field, also documented by the impressive efforts undertaken by the UNEDF SciDAC Collaboration [4, 5].

The application of DFT to the nuclear many-body problem has been very successful in recent years. Apart from conceptional advances aiming at, e. g., ab-initio studies of heavy nuclei, nuclear DFT studies provided us with a universal understanding of properties of nuclei which is relevant for a large variety of applications, see, e. g., Refs. [6–9] and also Ref. [10] for a review.

For some time, DFT approaches have been based on fitting the parameters of a given ansatz for the density functional such that one reproduces the experimentally determined values of the ground-state properties of various heavy nuclei [11]. The resulting density functionals have then been employed to describe ground-state properties of other heavy nuclei. In recent years, there have been many attempts to give microscopic constraints on the nuclear energy density functional employing, e. g., (improved) density matrix expansions [12, 13]. The latter approach has been further pursued and used to derive a (microscopic) nuclear energy density functional from chiral two- and three-nucleon interactions [14, 15]. On the other hand, the density-matrix expansion has been tested against ab initio calculations of trapped neutron drops [16]. These developments based on density-matrix expansions might be viewed as the beginning of a new era in the context of the nuclear energy density functional approach. Moreover, the future construction of density functionals will certainly benefit from various different approaches and complementary studies, ranging from a direct optimization of energy density functionals to studies of the equation of state of nuclear matter, see, e. g., Refs. [17–21]. At the present stage, however, our understanding of the constraints for energy density functionals emerging from microscopic nuclear forces as well as the (direct) relation of the energy density functional to these forces is not yet fully complete and requires further research. An ab-initio renormalization group (RG) approach to DFT could complement and extend these efforts [22, 23] since it may open up the possibility to directly compute ground-state properties of (heavy) nuclei from the underlying microscopic nucleon-nucleon interactions in a systematic fashion. In particular, such a functional RG approach seems to be promising since it allows to directly study the change of the energy density functional under 'RG transformations', e. g., from a weakly-interacting or even non-interacting system (starting point of the RG flow) to the fully interacting system, namely the nucleus under consideration [22, 23]. Moreover, such an RG approach is advantageous as it can be directly related to the underlying path integral for which many systematic approximation schemes are known, ranging from perturbative schemes to non-perturbative resummation techniques. For reviews and introductions to DFT approaches using the path-integral formalism, we refer the reader to Refs. [24, 25].

From a very field-theoretical point of view, the object of interest is the so-called (quantum) effective action which can be derived from the (exponentiated) path integral by introducing source terms and performing then a Legendre transformation with respect to theses sources, see also our discussion below. Such a construction is well-known in statistical physics where the Gibbs free energy of, e.g., a spin system, is computed from the underlying partition function by means of a Legendre transformation. In quantum field theory, it is possible to work along these lines and couple the sources to the (physically) rel-

evant "degrees of freedom". For DFT, this means that we couple the sources to the densities associated with the quantum fields and then perform a Legendre transformation with respect to these sources. The effective action resulting form such a procedure is, strictly speaking, called a two-particle point-irreducible (2PPI) effective action. This 2PPI effective action is directly related to the energy density functional introduced by Hohenberg and Kohn, see our discussion below and also Refs. [24, 25] for a review.

At this point, we have traced back the computation of the energy density functional to the computation of the path integral of the underlying theory defined by the microscopic interactions which itself represents an inherently difficult problem. Due to the relation of the energy density functional and the path integral, however, we can utilize powerful existing tools for the computation of the associated path integral. For example, we could employ *ab-initio* Monte-Carlo (MC) calculations or RG approaches. In the present work, we consider an RG approach to DFT that has been put forward in Refs. [22, 23]. For a more general discussion of the properties of nPPI effective actions, we refer the reader to Ref. [26].

In the present work, we give a detailed discussion of the RG approach to DFT introduced in Refs. [22, 23]. In Sect. II, we present a general discussion of the structure and properties of these DFT-RG flows, including their connection to perturbation theory as well as the Hartree and Hartree-Fock approximation. In Sect. III, we then apply our DFT-RG approach (2PPI-RG) approach to two simple toy models for which analytic solutions are known. In Sect. IV, we finally present our conclusions and outlook, including a concise discussion of our next steps towards an application our DFT-RG approach to the nuclear many-body problem.

II. RENORMALIZATION GROUP APPROACH TO DENSITY FUNCTIONAL THEORY

In this section, we give a more general discussion of field-theoretical aspects of the DFT-RG approach put forward in Ref. [22] and further discussed in Ref. [23].

A. RG flow equation

In nuclear DFT, we are particularly interested in strongly-interacting many-body systems (far) away from the continuum limit where the ground-state density is inhomogeneous.[1] More generally speaking, we aim at a study of a finite system of fermions interacting via a non-local interaction which may be repulsive at short distances and attractive at long range, as it is the case for the nuclear many-body problem and ultracold trapped Fermi gases. As discussed above, DFT has indeed proven to be useful for studies of these type of systems, see, e. g., Refs. [10, 27, 28].

Before we discuss the DFT-RG flow equation and its properties, we give a brief summary of the underlying principles of DFT. To this end, we restrict ourselves to the following action:[2]

$$S[\psi^\dagger,\psi] = \int_\tau \int_x \psi^\dagger_\sigma(\tau,\vec{x})\left[\partial_\tau - \Delta + V(\vec{x})\right]\psi_\sigma(\tau,\vec{x}) + \frac{1}{2}\int_\tau\int_x\int_y \psi^\dagger_\sigma(\tau,\vec{x})\psi^\dagger_{\sigma'}(\tau,\vec{y}\,')U(\vec{x},\vec{y})\psi_{\sigma'}(\tau,\vec{y}\,')\psi_\sigma(\tau,\vec{x})\,,$$

where we have set $2m = 1$ and introduced the shorthands $\int_\tau = \int_0^\beta d\tau$, $\int_x = \int d^dx$, d is the space dimension. The function $V(\vec{x})$ denotes a (background) potential. Moreover, we assume here and in the following that we sum over identical spin indices, if not stated otherwise. In the following we only consider two-body interactions. Higher-order N-body interactions will be ignored but can be included straightforwardly in our DFT-RG approach.

DFT is based on the famous *Hohenberg-Kohn theorem* [1]. For a given interaction potential U, this theorem states that there exists a one-to-one correspondence between the ground-state density and the potential $V(\vec{x})$ (up to an additive constant), at least for non-degenerate ground states. This implies that the ground-state density $n_{\rm gs}$ (uniquely) determines the ground-state wavefunction of the N-body problem under consideration. The latter can therefore be considered as a functional of the density n. Moreover, the expectation value of any physical observable is determined by a unique functional of the ground-state density. In particular, this is true for the ground-state energy of the system and implies the existence of an energy density functional $E[n]$. The ground-state density $n_{\rm gs}(\vec{x})$ can then be obtained by minimizing $E[n]$ with respect to the density:

$$E_{\rm gs} = \inf_n E[n]\,. \tag{1}$$

Moreover, it can be shown that the energy density functional in the limit of vanishing external potential V, the so-called *Hohenberg-Kohn* functional $E_{\rm HK}$, is *universal* for a *given* interaction potential U:

$$E_{\rm HK}[n] = E[n] - \int d^dx\, n(\vec{x})V(\vec{x})\,. \tag{2}$$

These considerations can be generalized to the case of degenerate ground states. However, we leave aside a discussion of the issue of V-representability, and also of N-representability, in the following. We refer the reader to, e. g., Refs. [29–31] for a more detailed discussion.

[1] Note that strong interactions are by no means necessary to induce inhomogeneous ground states. For example, the ground-state density of N non-interacting particles trapped in a harmonic oscillator potential is obviously inhomogeneous.

[2] Throughout this work, we use the imaginary-time formalism. The extent of the imaginary-time axis can then be identified with the inverse temperature $\beta = 1/T$.

The *Hohenberg-Kohn* theorem can be viewed as a starting point for an efficient description of many-body problems. However, the theorem does by no means provide a recipe for the computation of the *Hohenberg-Kohn* functional. Similar to the 1PI quantum effective action in conventional quantum field theory, the Hohenberg-Kohn functional consists of infinitely many terms. As we shall see below, the *Hohenberg-Kohn* functional is indeed closely related to a specific type of effective action. This observation implies that it is in general not possible to write down the exact *Hohenberg-Kohn* functional for a given many-body problem. Thus, an ansatz for the functional is required in order to determine the ground-state properties of a given many-body problem. Usually, it is difficult to find a systematic and stable approximation scheme. For example, the simplest approximation is the so-called local density approximation (LDA) which can be derived straightforwardly from the density dependence of the ground-state energy of the corresponding uniform many-body problem. The latter can, for instance, be computed with *ab-initio* MC simulations. It is indeed possible to show that LDA represents the lowest order in a systematic derivative expansion of the exact energy-density functional [32]. However, a low-order approximation of this type might only be justified in systems with weakly varying densities, such as ultracold Fermi gases with a large number of atoms in an isotropic trap [33]. For a general many-body problem, such a derivative expansion may have bad convergence properties.

Now we would like to make contact between DFT and the effective action approach to quantum field theory, see , e. g., Refs. [24, 25] for a more detailed introduction. The generating functional for our theory defined by the action S is given by[3]

$$Z[\{J_\sigma\}] \sim \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \, \mathrm{e}^{-S[\psi^\dagger,\psi]+\int_\tau \int_x J_\sigma(\tau,\vec{x})(\psi^\dagger_\sigma(\tau,\vec{x})\psi_\sigma(\tau,\vec{x}))} \equiv \mathrm{e}^{W[\{J_\sigma\}]} \,. \tag{3}$$

In contrast to the conventional textbook approach to quantum field theory, namely the 1PI formalism, we have coupled the external sources $\{J_\sigma\}$ to terms which are bilinear in the fermion fields.[4] These bilinears play the role of composite bosonic degrees of freedom.

Let us add a word on the issue of fixing the particle number in a path-integral approach. We can either introduce chemical potentials into the path integral to fix the numbers of the various particle species, say protons and neutrons, or we do not include chemical potentials but fix the particle numbers by choosing appropriate boundary conditions for the equations of motion, as discussed in Ref. [34]. In a concrete DFT-RG study, we shall follow the latter approach to fix the particle number [35].

We now introduce the so-called *classical* fields $\rho_\sigma(\tau,\vec{x})$ which are defined as the (functional) derivative of $W[\{J_\sigma\}]$ with respect to the corresponding sources $J_\sigma(\tau,\vec{x})$:

$$\rho_\sigma(\tau,\vec{x}) = \frac{\delta W[\{J_\sigma\}]}{\delta J_\sigma(\tau,\vec{x})} \,. \tag{4}$$

Note that ρ_σ is not only a function of τ and $\vec{x}$ but also a functional of the sources $\{J_\sigma\}$, i. e. $\rho_\sigma = \rho_\sigma[\{J_\sigma\}]$. Clearly, these fields are related to the particle densities. In complete analogy to the textbook derivation of the 1PI effective action, the 2PPI effective action is now defined as the Legendre transformation of W with respect to the sources J_σ:

$$\Gamma[\{\rho_\sigma\}] = \sup_{\{J_\sigma\}} \left\{ -W[\{J_\sigma\}] + \int_\tau \int_x J_\sigma(\tau,\vec{x})\rho_\sigma(\tau,\vec{x}) \right\} . \tag{5}$$

The so-defined 2PPI effective action $\Gamma[\{\rho_\sigma\}]$ determines completely the dynamics of the many-body problem and, up to a factor of β, it can be associated with the energy-density functional mentioned above in the context of the conventional *Hohenberg-Kohn* DFT formalism. We add that the exact equivalent of the energy density functional as introduced by Hohenberg and Kohn can be derived similarly, if one introduces time-independent sources $J_\sigma(\vec{x})$, see, e. g., Refs. [34, 36–38]. For a more general discussion on DFT in terms of a Legendre transformation, we refer the reader to Refs. [39, 40].

It is straightforward to show that the 2PPI effective action $\Gamma[\{\rho_\sigma\}]$ does not dependent on the sources $\{J_\sigma\}$:

$$\frac{\delta\Gamma[\{\rho_\sigma\}]}{\delta J_\sigma} = 0 \,. \tag{6}$$

On the other hand, we have

$$\frac{\delta\Gamma[\{\rho_\sigma\}]}{\delta\rho_\sigma(\tau,\vec{x})} = J_\sigma(\tau,\vec{x}) \,. \tag{7}$$

Thus, the ground-state configuration $\{\rho_{\sigma,\mathrm{gs}}\}$ is determined by this equation in the limit $J_\sigma \to 0$.[5] In other words, solving Eq. (7) for the fields $\rho_\sigma(\tau,\vec{x})$ in this limit, we find the ground-state configuration $\{\rho_{\sigma,\mathrm{gs}}\}$. We define the (time-independent) ground-state densities $n_{\mathrm{gs},\sigma}(\vec{x})$ as follows:

$$n_{\mathrm{gs},\sigma}(\vec{x}) := \frac{1}{\beta}\int_0^\beta d\tau \, \rho_{\mathrm{gs},\sigma}(\tau,\vec{x}) \,. \tag{8}$$

If the solutions $\{\rho_\sigma(\tau,\vec{x})\}$ turn out to be independent of the imaginary time τ, then we have $n_{\sigma,\mathrm{gs}}(\vec{x}) \equiv \rho_{\sigma,\mathrm{gs}}(\tau,\vec{x})$.

[3] Here, we have dropped an irrelevant normalization factor of the path integral.

[4] Note that the formalism can be generalized by including sources coupled to, e. g., pairing densities. The latter might be considered as convenient effective degrees of freedom to describe the ground-state properties of certain many-body systems.

[5] In the limit of vanishing sources, Eq. (7) represents the quantum equation of motion of the composite degrees of freedom ρ_σ.

In our toy model studies to be discussed below, this is indeed the case.[6]

From the solutions $\{\rho_\sigma(\tau,\vec{x})\}$, we eventually obtain the ground-state energy $E_{\rm gs}$ of the system:

$$E_{\rm gs} := \lim_{\beta\to\infty} \frac{1}{\beta}\Gamma[\{\rho_{\sigma,{\rm gs}}\}]\,. \tag{9}$$

This relation follows immediately from the spectral representation of the partition function Z: $Z \sim \sum_n {\rm e}^{-\beta E_n}$, and $\Gamma \sim -W[J]|_{\{J_\sigma\to 0\}} \sim \ln Z[J]|_{\{J_\sigma\to 0\}}$. From Eq. (9), we can also anticipate the relation between the effective action Γ and the *Hohenberg-Kohn* functional $E_{\rm HK}$: $\Gamma \sim \beta E_{\rm HK}$.

At this point, we would like to add that the *universality* of the *Hohenberg-Kohn* functional $E_{\rm HK}$ follows from the fact that background potential can be absorbed into the source terms J_σ by a simple shift, $J_\sigma \to J_\sigma + V$, see Ref. [22]. Exploiting this observation, we find

$$\Gamma[\{\rho_\sigma\}] = \Gamma_{\rm HK}[\{\rho_\sigma\}] + \sum_\sigma \int_0^\beta d\tau \int d^dx\, V(\vec{x})\rho_\sigma(\tau,\vec{x})\,, \tag{10}$$

where $\Gamma_{\rm HK}[\{\rho_\sigma\}] = \Gamma_{V=0}[\{\rho_\sigma\}]$. We conclude that the functional $\Gamma_{\rm HK}[\{\rho_\sigma\}]$ depends only on our choice for the interaction potential but not on the background potential V. Recall that in our case the ρ_σ's depend in general on the imaginary time τ, in contrast to the standard *Hohenberg-Kohn* functional which depends only on a time-independent density. In this respect, our present argument can be viewed as a trivial generalization of the original universality argument given by Hohenberg and Kohn.

As discussed above, the computation of the effective action Γ ($\sim$ *Hohenberg-Kohn* functional) for a given theory can be an inherently difficult task. In the present work, we employ a DFT-RG approach that has been put forward in Refs. [22, 23, 38]. For details on the derivation, we also refer the reader to these papers. For convenience, we only consider a system of N spinless fermions in the following. However, we stress that the derivation of the flow equation is by no means bound to such a theory but can be straightforwardly generalized to other non-relativistic theories. To be more specific, we consider a classical action of the following general form:

$$S_\lambda[\psi^*,\psi] = \int_\tau\int_x \psi^*(\tau,\vec{x})\left[\partial_\tau - \Delta + V_\lambda(\vec{x})\right]\psi(\tau,\vec{x}) + \frac{\lambda}{2}\int_\tau\int_x\int_{\tau'}\int_{x'} \psi^*(\tau,\vec{x})\psi^*(\tau',\vec{x}')U(\tau,\tau';\vec{x},\vec{x}')\psi(\tau',\vec{x}')\psi(\tau,\vec{x})$$

with $2m \equiv 1$. Here, we allow for a very general form of the two-body interaction. In most cases, however, one will restrict U to be of the form $U \sim \delta(\tau-\tau')\tilde{U}(\vec{x},\vec{x}')$. The parameter $\lambda \in [0,1]$ denotes a dimensionless control parameter: For $\lambda = 0$, the two-body interaction potential U is turned off and we are left with an exactly soluble non-interacting problem, namely N fermions trapped in a given potential V_λ. For $\lambda = 1$, the potential U is fully turned on and the potential V_λ has assumed its physical form. For example, V_λ can be chosen such that it plays the role of the trap potential in an experiment with ultracold Fermi gases. In studies of ground-state properties of self-bound many-body problems, such as nuclei, one chooses $V_{\lambda=1}(\vec{x}) \equiv 0$. Apart from the physical constraint at $\lambda = 1$, the form of V_λ is at our disposal and can be chosen such that, e. g., the initial non-interacting problem is simple to solve. For example, we could choose $V_{\lambda=0}$ to be a harmonic potential.

We add that, from a field-theoretical point of view, the one-body potential V_λ acts as a regulator function. In fact, the length scale associated with the potential V_λ sets a momentum scale in the theory which removes infrared divergences in the appearing loop diagrams. In this sense, the introduction of the parameter λ renders the theory scale-dependent. In particular for the case $V_{\lambda=1}(\vec{x}) \equiv 0$, we shall also assume that the Fourier transform of the interaction potential U falls off sufficiently rapidly for large momenta to avoid the occurrence of ultraviolet divergences.

Following Refs. [22, 23], it is now straightforward to derive the RG flow equation for the 'scale-dependent' 2PPI effective action $\Gamma_\lambda[\rho]$. By taking the derivative of $\Gamma_\lambda[\rho]$ with respect to λ, we find

$$\partial_\lambda\Gamma_\lambda[\rho] = (\partial_\lambda V_\lambda)\cdot\rho + \frac{1}{2}\rho\cdot U\cdot\rho + \frac{1}{2}\,{\rm Tr}\, U\cdot\left(\frac{\delta^2\Gamma_\lambda[\rho]}{\delta\rho\delta\rho}\right)^{-1}, \tag{11}$$

where the dot represents a shorthand for

$$A\cdot B \equiv \int_0^\beta d\tau\int d^dx A(\tau,\vec{x})B(\tau,\vec{x}) \tag{12}$$

and the trace Tr stands for

$${\rm Tr}\, M(\tau',\vec{x}',\tau,\vec{x}) = \int_0^\beta d\tau\int d^dx M(\tau,\vec{x},\tau,\vec{x})\,. \tag{13}$$

This functional differential equation (11) describes the flow from the non-interacting system defined at $\lambda = 0$ to the interacting theory defined at the physical point $\lambda = 1$. The effective action $\Gamma_{\lambda=0}[\rho]$ associated with an exactly

[6] In fact, this τ-independence of $\rho_{\rm gs}$ follows from our flow equation (11) to be discussed below, provided that we only consider an interaction potential U with a imaginary-time dependence of the form $U \sim \delta(\tau-\tau')$.

soluble (non-interacting) N-body problem determines the initial condition of the RG flow.

In the terminology of many-body physics, the second term in Eq. (11) can be identified as the so-called Hartree term. The third term on the right-hand side depends on the scale-dependent density-density correlator $\delta^2\Gamma_\lambda[\rho]/(\delta\rho\delta\rho)$ and includes all other corrections to the effective action, also so-called Fock contributions, see also our discussion in Sect. II D.

We observe that the flow equation (11) has a simple one-loop structure as it is the case for the RG flow equation for the 1PI effective action derived by Wetterich [41, 42]. However, this does not mean that we can only capture one-loop corrections with this flow equation. On the contrary, by solving the functional differential equation (11), we automatically include corrections of arbitrarily high-order, see also our discussion in Sect. II C. In fact, no approximations are involved in the derivation of the flow equation (11). In particular, the derivation of this flow equation does not require that the interaction strength is small. The equation is exact, provided we only allow for two-body interactions in the classical action S_λ.[7]

For a general many-body problem, it is not possible to solve the flow equation (11) for the 2PPI effective action (corresponding to the *Hohenberg-Kohn* functional) exactly. Thus, we need to find (systematic) approximation/truncation schemes. Examples for such approximation schemes are the gradient expansion of the effective action or an expansion of $\Gamma_\lambda[\rho]$ about the ground state $\rho_{\mathrm{gs},\lambda}$:

$$\Gamma_\lambda[\rho] = \Gamma_\lambda[\rho_{\mathrm{gs},\lambda}] + \frac{1}{2}\int_\tau\int_x\int_{\tau'}\int_{x'} \left(\rho(\tau,\vec{x}) - \rho_{\mathrm{gs},\lambda}(\tau,\vec{x})\right)\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}](\tau,\vec{x};\tau',\vec{x}')\left(\rho(\tau',\vec{x}') - \rho_{\mathrm{gs},\lambda}(\tau',\vec{x}')\right) + \dots . \quad (14)$$

Plugging this expansion into the general flow equation (11), we obtain the flow equations for $\Gamma_\lambda[\rho_{\mathrm{gs},\lambda}]$, $\rho_{\mathrm{gs},\lambda}$, and $\Gamma_\lambda^{(n)}[\rho_{\mathrm{gs},\lambda}]$ with $n \geq 2$. We then find that the flow of $\rho_{\mathrm{gs},\lambda}$ depends on $\rho_{\mathrm{gs},\lambda}$ itself but also on $\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}]$ and $\Gamma_\lambda^{(3)}[\rho_{\mathrm{gs},\lambda}]$. The flow equation for the two-point function $\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}]$ depends on $\rho_{\mathrm{gs},\lambda}$, $\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}]$, $\Gamma_\lambda^{(3)}[\rho_{\mathrm{gs},\lambda}]$, and $\Gamma_\lambda^{(4)}[\rho_{\mathrm{gs},\lambda}]$. In general, we find that the flow of $\Gamma_\lambda^{(n)}[\rho_{\mathrm{gs},\lambda}]$ depends on $\rho_{\mathrm{gs},\lambda}$ and $\Gamma_\lambda^{(m)}[\rho_{\mathrm{gs},\lambda}]$ with $m = 2,\dots,n,n+1,n+2$.

In the terminology of quantum field theory, the expansion (14) corresponds to a vertex expansion and will be discussed in detail in our toy model studies in Sect. III. Loosely speaking, the n-point correlation function is related to the expectation value of n density operators:

$$\Gamma_\lambda^{(n)}[\rho_{\mathrm{gs},\lambda}](\tau_1,\vec{x}_1;\dots;\tau_n,\vec{x}_n) \sim \langle\hat{\rho}(\tau_1,\vec{x}_1)\hat{\rho}(\tau_2,\vec{x}_2)\cdots\hat{\rho}(\tau_n,\vec{x}_n)\rangle_{\mathrm{gs}}\,, \quad (15)$$

where

$$\hat{\rho}(\tau,\vec{x}) = \psi^*(\tau,\vec{x})\psi(\tau,\vec{x})\,. \quad (16)$$

For brevity, we have dropped the subtraction of the disconnected contributions on the right-hand side of Eq. (15), see Eq. (19) for a more rigorous expression for $n = 2$. At this point, we would like to stress that the vertex expansion given in Eq. (14) is an exact expansion of the functional $\Gamma_\lambda[\rho]$ about the ground state and should by no means be confused with the local density approximation. Recall that the expansion coefficients, namely the n-point functions, are functions of the time-like and spatial coordinates.

Before we discuss the features of our RG flow equation, we would like to emphasize that our present approach allows us to directly compute the energy density functional from the microscopic interactions of the theory. To be concise, it opens up the possibility to derive the energy density functional (and the ground-state properties) of, say, heavy nuclei from chiral effective field theory interactions [43–47] as the latter can be used to determine the interaction potential U in our flow equation.

B. Excited States

Up to this point, we have only discussed how to compute the ground-state energy. However, it is also possible to extract the energy of the excited states of the theory from the 2PPI effective action $\Gamma[\{\rho_\sigma\}] \equiv \Gamma_{\lambda=1}[\{\rho_\sigma\}]$. To this end, it comes to our rescue that we consider the system at a finite temperature T. Using now the spectral representation of the partition function Z, we find

$$\Gamma[\{\rho_{\sigma,\mathrm{gs}}\}] = -\ln\left(\sum_n \mathrm{e}^{-\beta E_n}\right) + \text{const.}\,. \quad (17)$$

In order to obtain the energy of the excited states E_n ($n > 0$, $E_{\mathrm{gs}} \equiv E_0$), we could simply compute $\Gamma[\{\rho_{\sigma,\mathrm{gs}}\}]$ as a function of β and then fit the result to the functional form given on the right-hand side of Eq. (17) with the energies of the excited states E_n as the free fit parameters. For sufficiently low temperatures (i. e. sufficiently large β), it is reasonable to assume that only the

[7] A generalization of this flow equation to include the effects of higher n-body operators is straightforward. In principle, this requires to also multiply the 3−, 4−, ... body-interaction terms with the control parameter λ.

lowest-lying states are occupied. In a fit, we would then only include a small finite number of fit parameters corresponding to these states. However, such a procedure may still turn out to be impractical from a numerical point of view.

In order to extract the energy of the first excited state, we do not require a fit procedure involving the spectral representation of the partition function. In fact, the first excited state E_1 can be extracted from the two-density correlation function evaluated at the ground state,

$$\Gamma^{(2)}_{\sigma,\sigma'}(\tau,\vec{x};\tau',\vec{x}')\Big|_{\{\rho_{\sigma,\mathrm{gs}}\}} = \frac{\delta^2\Gamma[\{\rho_\sigma\}]}{\delta\rho_\sigma(\tau,\vec{x})\delta\rho_{\sigma'}(\tau',\vec{x}')}\bigg|_{\{\rho_{\sigma,\mathrm{gs}}\}} .$$

First, we note that $\Gamma^{(2)}_{\sigma,\sigma'}$ is directly related to the (field-dependent) propagator $G_{\sigma,\sigma'}$:

$$G_{\sigma,\sigma'}(\tau,\vec{x};\tau',\vec{x}') = \left(\Gamma^{(2)}_{\sigma,\sigma'}(\tau,\vec{x};\tau',\vec{x}')\right)^{-1} . \quad (18)$$

On the other hand, the propagator can be written in terms of expectation values of density operators:

$$G_{\sigma,\sigma'}(\tau,\vec{x};\tau',\vec{x}') = \langle\hat{\rho}_\sigma(\tau,\vec{x})\hat{\rho}_{\sigma'}(\tau',\vec{x}')\rangle - \langle\hat{\rho}_\sigma(\tau,\vec{x})\rangle\,\langle\hat{\rho}_{\sigma'}(\tau',\vec{x}')\rangle . \quad (19)$$

The quantity $\hat{\rho}_\sigma$ is the straightforward generalization of $\hat{\rho}$ defined in Eq. (16). From this expression, it follows that

$$(E_1 - E_{\mathrm{gs}}) = -\lim_{\beta\to\infty}\frac{1}{\beta}\ln G_{\sigma,\sigma}(0,\vec{x};\beta,\vec{x}') , \quad (20)$$

independent of our choice for the space-time coordinate-pairs $(\tau,\vec{x})$ and $(\tau',\vec{x}')$. Thus, we can extract the energy of the first excited state from the knowledge of the two-point correlation function once we have computed the ground-state energy using Eq. (9). In principle, it is also possible to project on higher-lying excited states by considering the expectation values of properly chosen operators. In any case, our discussion shows that excited states are also accessible within our 2PPI effective action approach.

C. Perturbation Theory

Let us now discuss the properties of our DFT-RG approach in more detail. For convenience, we now restrict ourselves again to the case of spinless fermions, i. e. we shall consider the flow equation (11) in the following. However, our line of arguments also holds for any type of fields: fermions with spin or even scalar fields as we shall see in our toy model studies in Sect. III.

In order to recover perturbation theory from the flow equation (11), we first introduce a counting parameter u_0 into the theory as follows:

$$U(\tau,\tau';\vec{x},\vec{x}') = u_0\tilde{U}(\tau,\tau';\vec{x},\vec{x}') , \quad (21)$$

where

$$\tilde{U}(\tau,\tau';\vec{x},\vec{x}') = \phi_{\mathrm{U}}(\vec{x},\vec{x}')\delta(\tau-\tau') . \quad (22)$$

Here, the full dependence on the space coordinates has been absorbed into the function ϕ_{U}. For convenience, we assume that the dependence on the imaginary time is given by $\delta(\tau-\tau')$ and that ϕ_{U} is a dimensionless function. Now we can introduce a dimensionless counting parameter $\bar{u}_0$,

$$\bar{u}_0 = \ell_V^2 u_0 . \quad (23)$$

Here, ℓ_V denotes a typical length scale associated with the background potential V. For example, we have $\ell_V = 1/\sqrt{\omega}$, if we choose a harmonic background potential: $V(\vec{x}) = (1/2)\omega^2\vec{x}^{\,2}$. Using the length scale ℓ_V, we can also introduce the dimensionless ground-state energy, density, as well as dimensionless correlation functions $\Gamma^{(n)}_\lambda$:

$$\bar{E}_{\mathrm{gs}} = \ell_V^2 E_{\mathrm{gs}} , \qquad \bar{\rho}_{\mathrm{gs}} = \ell_V^d\rho_{\mathrm{gs}} , \quad (24)$$

and

$$\bar{\Gamma}^{(n)} = \ell_V^{2n}\Gamma^{(n)} , \quad (25)$$

where $\Gamma^{(n)} = \delta^n\Gamma/\delta\rho^n$. Note that $\ell_V^{-2}\beta$ is dimensionless.

The dimensionless ground-state energy, density, and correlation functions can be expanded in powers of $\bar{u}_0$:

$$\bar{E}_{\mathrm{gs}} = \sum_{n=0}^{\infty}\epsilon_n\bar{u}_0^n , \quad (26)$$

$$\bar{\rho}_{\mathrm{gs}} = \sum_{n=0}^{\infty}\nu_n\bar{u}_0^n , \quad (27)$$

$$\bar{\Gamma}^{(m)} = \sum_{n=0}^{\infty}\gamma_n^{(m)}\bar{u}_0^n . \quad (28)$$

The coefficients ϵ_0, ν_0, and $\gamma_0^{(m)}$ are determined by the initial condition of the flow equation, i. e. by the functional $\Gamma_{\lambda=0}$ of the non-interacting theory. At $\lambda = 0$, all the expansion coefficients with $n > 0$ are identical to zero. However, all the coefficients ϵ_n, ν_n, and $\gamma_n^{(m)}$ with $n > 0$ depend implicitly on λ and may therefore be generated dynamically by quantum corrections. Note that the coefficients ν_n also depend on τ and $\vec{x}$. Analogously, the coefficients $\gamma_n^{(m)}$ depend on m pairs $(\tau,\vec{x})$ of space-time coordinates.

Let us now analyze the perturbative expansion of the ground-state energy. To this end, we apply the expansion (14) about the current ground-state to our general flow equation (11). This yields the following equation for $\Gamma_\lambda[\rho_{\mathrm{gs}}]$:

$$\partial_\lambda\Gamma_\lambda[\rho_{\mathrm{gs},\lambda}] = (\partial_\lambda V_\lambda)\cdot\rho_{\mathrm{gs},\lambda} + \frac{1}{2}\rho_{\mathrm{gs},\lambda}\cdot U\cdot\rho_{\mathrm{gs},\lambda} + \frac{1}{2}\,\mathrm{Tr}\,U\cdot\left(\frac{\delta^2\Gamma_\lambda[\rho]}{\delta\rho\delta\rho}\bigg|_{\rho_{\mathrm{gs},\lambda}}\right)^{-1} . \quad (29)$$

Plugging the expansions (26)-(28) into this flow equation and noting that $E_{\mathrm{gs},\lambda} = \Gamma[\rho_{\mathrm{gs},\lambda}]/\beta$ for $\beta\to\infty$, we can derive flow equations for the coefficients ϵ_n by simply

comparing the left-hand side and right-hand side order by order in our expansion in powers of $\bar{u}_0$.

Let us now distinguish between two cases, namely the case with a λ-dependent background potential and the one with a λ-independent background potential. We begin our analysis with the latter case. The first term on the right-hand side of Eq. (29) then vanishes identically. To the flow of the coefficient ϵ_0, no term on the right-hand side of Eq. (29) contributes since they depend explicitly on the interaction potential. Thus, these terms can only contribute to the flow of the coefficients ϵ_n with $n > 0$.

In order to obtain the correct result for the ground-state energy E_{gs} ($\sim \Gamma[\rho_{\mathrm{gs}}]$) in leading order in $\bar{u}_0$, we deduce from Eq. (11) that we need to compute the coefficient $\gamma_0^{(2)}$ which is associated with the term independent of $\bar{u}_0$ in the expansion (28):

$$\mathrm{Tr}\, U \cdot \left(\frac{\delta^2 \Gamma_\lambda[\rho]}{\delta\rho\delta\rho}\bigg|_{\rho_{\mathrm{gs},\lambda}} \right)^{-1} \sim \bar{u}_0\, \mathrm{Tr}\, \tilde{U} \cdot \left(\gamma^{(2)}\right)^{-1} + \mathcal{O}(\bar{u}_0^2)\,.$$

Interaction-induced corrections of the propagator do not contribute to the leading-order correction of the ground-state energy. This follows immediately from the fact that the third term on the right-hand side of Eq. (29) depends explicitly on the interaction potential U and therefore on $\bar{u}_0$. Since the second term on the right-hand side has an explicit U-dependence as well, the coefficient ν_0 is also required to recover the result from perturbation theory at leading order:

$$\rho_{\mathrm{gs},\lambda} \cdot U \cdot \rho_{\mathrm{gs},\lambda} \;\sim\; \bar{u}_0 \left(\nu_0 \cdot \tilde{U} \cdot \nu_0\right) + \mathcal{O}(\bar{u}_0^2)\,.$$

These considerations can be continued successively. In general, we find that we need to compute ρ_{gs} and the two-point function up to order $\bar{u}_0^{n-1}$, in order to obtain the correct result for the ground-state energy up to order $\bar{u}_0^n$.

Let us now turn to the case with a λ-dependent background potential. We can follow the same line of arguments as in the previous case. Due to the presence of the term $(\partial_\lambda V_\lambda)\cdot\rho_{\mathrm{gs},\lambda}$, however, we now find that we need to compute $\rho_{\mathrm{gs},\lambda}$ and the two-point function up to order $\bar{u}_0^n$ in order to obtain the correct result for the ground-state energy up to order $\bar{u}_0^n$.[8]

In summary, we have seen that the computation of the ground-state energy up to a given order $\bar{u}_0$ requires that we also compute ρ_{gs} and the two-point function up to a certain order. The required expansion order for the latter depends on whether the background potential is λ-dependent or not.

As already mentioned above, the flow equations for the density and the two-point function (and therewith for their expansion coefficients) can be obtained by expanding the general flow equation (11) about the current ground state $\rho_{\mathrm{gs},\lambda}$ and then projecting it on the corresponding quantities, namely $\Gamma_\lambda[\rho_{\mathrm{gs},\lambda}]$, $\rho_{\mathrm{gs},\lambda}$, and the n-point correlation functions $\Gamma_\lambda^{(n)}[\rho_{\mathrm{gs},\lambda}]$, see also Eq. (14). We shall discuss this procedure in great detail in our toy model studies in Sect. III. At this point, however, we already would like to emphasize that the vertex expansion should by no means be confused with the perturbative series expansion discussed above. The associated expansion coefficients are inherently non-perturbative quantities. Below, we use the vertex expansion about the current ground-state since it is systematic and allows us to extract the RG equations for $\Gamma_\lambda[\rho_{\mathrm{gs},\lambda}]$, $\rho_{\mathrm{gs},\lambda}$, and the n-point correlation functions $\Gamma_\lambda^{(n)}[\rho_{\mathrm{gs},\lambda}]$ in a simple manner.

D. Hatree approximation

The so-called Hartree approximation can be obtained from the general flow equation (11) by dropping the third term on the right-hand side. The latter includes, e. g., the so-called Fock term. Dropping the third term on the right-hand side of Eq. (11), we can solve the flow equation for $\Gamma_\lambda[\rho]$ analytically. We find

$$\Gamma_\lambda[\rho] = (V_\lambda - V_{\lambda=0})\cdot\rho + \frac{\lambda}{2}\rho\cdot U\cdot\rho + \Gamma_{\lambda=0}[\rho]\,, \quad (30)$$

where $\Gamma_{\lambda=0}[\rho]$ is simply the 2PPI effective action of the non-interacting (initial) system at $\lambda = 0$. From the definition of the ground-state,

$$\frac{\delta\Gamma_\lambda[\rho]}{\delta\rho}\bigg|_{\rho_{\mathrm{gs},\lambda}} = 0\,, \quad (31)$$

we obtain the implicit equation

$$\rho_{\mathrm{gs},\lambda} = -\frac{2}{\lambda}\, U^{-1}\cdot\left[\Delta V_\lambda + \frac{\delta\Gamma_{\lambda=0}[\rho]}{\delta\rho}\bigg|_{\rho_{\mathrm{gs},\lambda}}\right] \quad (32)$$

with $\Delta V_\lambda = (V_\lambda - V_{\lambda=0})$. Expanding the initial effective action $\Gamma_{\lambda=0}[\rho]$ about the initial ground-state $\rho_{\mathrm{gs},0} \equiv \rho_{\mathrm{gs},\lambda=0}$ only up to second order, we find the following solution for $\rho_{\mathrm{gs},\lambda}$:

$$\rho_{\mathrm{gs},\lambda} = -\left[\frac{\lambda}{2}U + \Gamma^{(2)}_{\mathrm{gs},0}\right]^{-1}\cdot\left[\Delta V_\lambda - \Gamma^{(2)}_{\mathrm{gs},0}\cdot\rho_{\mathrm{gs},0}\right]\,, \quad (33)$$

where $\Gamma^{(2)}_{\mathrm{gs},0} := \Gamma^{(2)}_{\mathrm{gs},\lambda=0}[\rho_{\mathrm{gs},\lambda=0}]$. However, such a low-order expasion in ρ can only be meaningful if the interacting ground-state $\rho_{\mathrm{gs},\lambda=1}$ is close to the initial non-interacting ground-state $\rho_{\mathrm{gs},\lambda=0}$. In general, it is difficult

[8] In fact, this case is more subtle. Whereas it is apparent that we have to compute ρ_{gs} up to order $\bar{u}_0^n$ in order to obtain the correct result for the ground-state energy to the same order, one might naively expect that we only need to compute the two-point function up to order $\bar{u}_0^{n-1}$, as in the previous case. However, the computation of ρ_{gs} up to order $\bar{u}_0^n$ requires that we know the two-point function up to order $\bar{u}_0^n$, in the case of a λ-dependent background potential. Overall, we therefore need to compute ρ_{gs} and the two-point function up to order $\bar{u}_0^n$ in order to obtain the correct result for the ground-state energy up to this order.

to judge *a priori* whether this is the case.[9] From a practical point of view, we therefore have to include higher orders in the expansion of $\Gamma_{\lambda=0}[\rho]$ and analyze the convergence of the physical observables as a function of the expansion order.

From our discussion, it follows that the Hartree approximation already yields arbitrarily high orders in an expansion in powers of $\bar{u}_0$, both for the ground-state energy and density. Recall that $U \sim \bar{u}_0$ and $E_{\rm gs} \sim \Gamma[\rho_{\rm gs}]$. However, we would like to point out a shortcoming of the Hartree approximation which becomes apparent from our analysis. Taking into account our findings from Sect. II C, we conclude that the Hartree approximation necessarily fails to reproduce the perturbative result for the ground-state energy, even at leading order. This is simply due to the fact that the third term on the right-hand side of Eq. (11) is missing in this approximation. This term depends explicitly on the interaction potential. Since $\delta^2\Gamma_\lambda/(\delta\rho\delta\rho)$ is in general not identical to zero, even in the non-interacting limit, this term generates terms which already contribute to the leading order in a perturbative expansion.

III. CASE STUDIES

In this work, we refrain from an explicit study of ground-state properties of nuclei but rather present toy model studies to explain the theoretical formalism detailed in the previous section. The (classical) actions S underlying our toy model studies resemble the action underlying non-relativistic many-body problems in a few aspects, at least from a purely field-theoretical point of view. However, we also would like to emphasize that such toy model studies only represent a first step. Studies of simple self-bound many-body models, which are also much closer to nuclear physics from a phenomenological point of view, will be presented elsewhere [35].

A. Zero-dimensional Toy Model

The simplest example for the application of our RG approach is the computation of 'ordinary' integrals which, loosely speaking, corresponds to zero-dimensional field theory. In this case, the partition function corresponding to Eq. (3) is an 'ordinary' integral of the form[10]

$$Z[J] \sim \int_{-\infty}^{\infty} d\psi \, \mathrm{e}^{-S[\psi]+J\psi^2} \,, \tag{34}$$

[9] Strictly speaking, the notion 'close' requires the definition of a measure on the space defined by the functions ρ. We shall skip this issue here.

[10] Here and in the following, we drop again irrelevant normalization factors of the partition function. Moreover, we note that the quantities $Z[J]$, $\Gamma[\rho]$, ... are no functionals but 'ordinary' functions in the present case. Nevertheless, we stick to our notation introduced in the previous section.

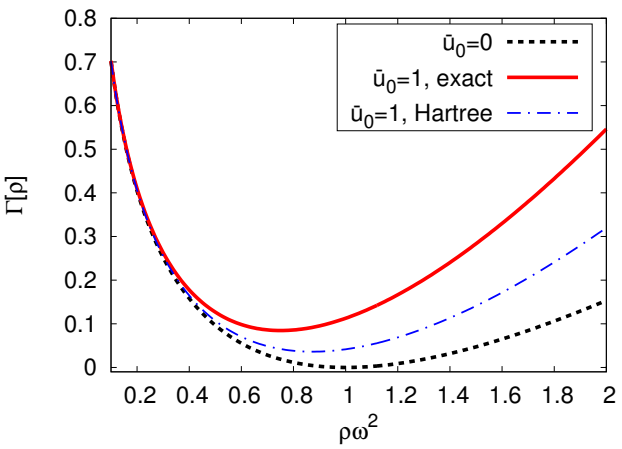

Figure 1. Effective action $\Gamma[\rho]$ of the zero-dimensional toy model for the non-interacting case $\bar{u}_0 = 0$ and for $\bar{u}_0 = 1$, as obtained from a direct calculation of the partition function. We have normalized the effective action such that $\Gamma[\rho_{\rm gs}] = 0$ for $\bar{u}_0 = 0$.

where

$$S[\psi] = \frac{1}{2}\omega^2\psi^2 + \frac{u_0}{24}\psi^4 \,. \tag{35}$$

Here, J and ψ are real-valued numbers rather than fields. Thus, the derivative terms in the action vanish identically. Moreover, we have chosen $U = u_0/12$ for the interaction potential and $V_\lambda = (1/2)\omega^2$ for the background potential. We add that zero-dimensional models have been already successfully employed to benchmark other field-theoretical methods, see, e. g., Ref. [48].

For $\bar{J} = J/\omega^2 \leq -1/2$, the partition function can be given in closed form:

$$Z[\bar{J}] \sim \frac{\sqrt{3-6\bar{J}}\, K_{\frac{1}{4}}\left(\frac{3(1-2\bar{J})^2}{4\bar{u}_0}\right) \mathrm{e}^{\frac{3(1-2\bar{J})^2}{4\bar{u}_0}}}{\sqrt{\bar{u}_0}} \equiv \mathrm{e}^{W[J]}, \tag{36}$$

where $\bar{u}_0 = u_0/\omega^4$ and K_ν is the modified Bessel function of the second kind of order ν, see, e. g., Ref. [49]. For $\bar{J} > -1/2$, the integral $Z[J]$ can still be computed numerically.

Using Eq. (4) and taking the limit $J \to 0$, we can now compute the ground-state $\rho_{\rm gs} \equiv \langle\psi^2\rangle_{\rm gs}$:

$$\rho_{\rm gs} = \left(\omega^2\bar{u}_0 K_{\frac{1}{4}}\left(\frac{3}{4\bar{u}_0}\right)\right)^{-1}\left((\bar{u}_0+3)K_{\frac{1}{4}}\left(\frac{3}{4\bar{u}_0}\right) - \frac{3}{2}K_{\frac{5}{4}}\left(\frac{3}{4\bar{u}_0}\right) - \frac{3}{2}K_{-\frac{3}{4}}\left(\frac{3}{4\bar{u}_0}\right)\right) . \tag{37}$$

This expression can be expanded in powers of $\bar{u}_0$:

$$\rho_{\rm gs} = \omega^{-2}\left(1 - \frac{\bar{u}_0}{2} + \frac{2\bar{u}_0^2}{3} - \frac{11\bar{u}_0^3}{8} + \mathcal{O}\left(\bar{u}_0^4\right)\right) . \tag{38}$$

The ground-state 'energy' can be obtained directly from

$$E_{\rm gs} = -\left(\ln Z[0] - \ln Z[0]\big|_{u_0\to 0}\right) , \tag{39}$$

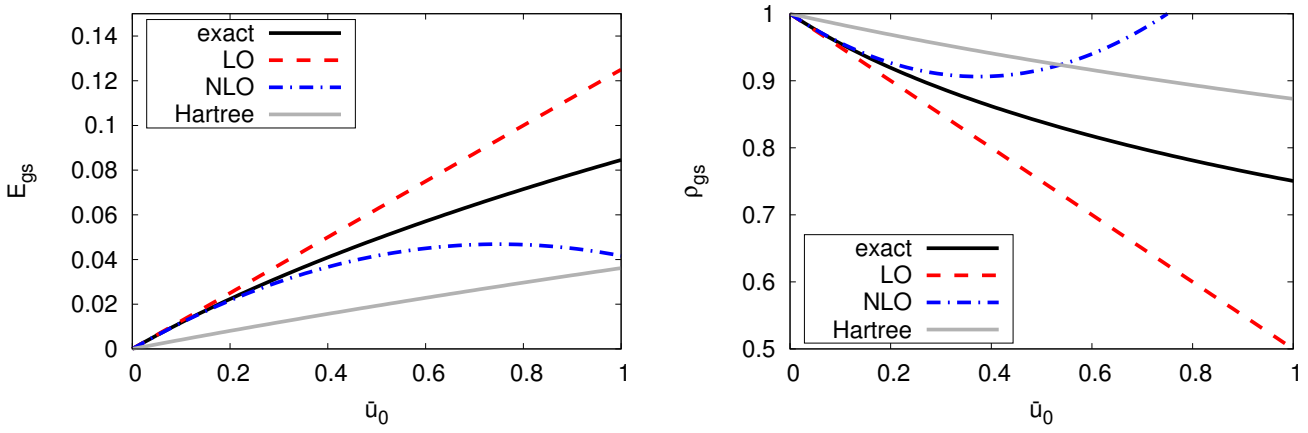

Figure 2. Ground-state 'energy' $E_{\rm gs}$ and ground-state 'density' $\rho_{\rm gs}$ of the zero-dimensional toy model as a function of the (dimensionless) coupling $\bar{u}_0$. For comparison, we also show the results from a small coupling expansion at leading order (LO) and next-to-leading order (NLO).

where we have normalized $E_{\rm gs}$ such that it is zero for $\bar{u}_0 \to 0$. For small $\bar{u}_0$, we find

$$E_{\rm gs} = \frac{\bar{u}_0}{8} - \frac{\bar{u}_0^2}{12} + \frac{11\bar{u}_0^3}{96} + \mathcal{O}\left(\bar{u}_0^4\right) . \tag{40}$$

Alternatively, we may compute the effective action $\Gamma[\rho]$ using Eq. (5). From the minimization of the effective action, we then obtain $\rho_{\rm gs}$ and $E_{\rm gs}$. Note that the computation of the effective action requires that we solve $\rho \equiv \rho[J]$, as defined by Eq. (4), for the source J. The solution $J = J[\rho]$ needs to be plugged into the definition (5) of the effective action. For the case $\bar{u}_0 = 0$, for instance, the effective action can be computed analytically. We find

$$\Gamma_{\bar{u}_0=0}[\rho] = \frac{1}{2}\left(\rho\omega^2 - \ln\left(2\pi\rho\omega^2\right) - 1\right) . \tag{41}$$

Apparently, any global analytic ansatz for $\Gamma_{\bar{u}_0=0}$ is bound to fail. However, a Taylor expansion about the ground-state $\rho_{\rm gs}\omega^2 = 1$ (for $\bar{u}_0 = 0$) is possible and meaningful.

For $\bar{u}_0 > 0$, the computation of the effective action can only be performed numerically. We find that the non-analyticity at $\rho = 0$ persists in this case. In Fig. 1 we show the effective action $\Gamma[\rho]$ as a function of ρ for $\bar{u}_0 = 1$. We have normalized $\Gamma[\rho]$ such that $\Gamma[\rho_{\rm gs}] = 0$ for $\bar{u}_0 = 0$. For $\bar{u}_0 = 1$, the ground state $\rho_{\rm gs}$ is found at $\rho_{\rm gs} = 0.750\ldots$, in agreement with our analytic result (37). For the ground-state 'energy', we find $E_{\rm gs} = 0.084\ldots$, which also agrees with the analytically found value as obtained from Eqs. (36) and (39). We can compare these results with those from the effective action in the Hartree approximation as derived from Eq. (30):

$$\Gamma_{\rm Hartree}[\rho] = \frac{\bar{u}_0}{24}(\rho\omega^2)^2 + \Gamma_{\bar{u}_0=0}[\rho] + \frac{1}{2}\ln(2\pi) . \tag{42}$$

The normalization has been again chosen such that $\Gamma_{\rm Hartree}[\rho_{\rm gs,Hartree}] = 0$ for $\bar{u}_0 \to 0$. For the ground-state, we find

$$\begin{aligned}\rho_{\rm gs,Hartree}(\bar{u}_0) &= \bar{u}_0^{-1}\left(\sqrt{6\bar{u}_0 + 9} - 3\right) \\ &= 1 - \frac{\bar{u}_0}{6} + \frac{\bar{u}_0^2}{18} - \frac{5\bar{u}_0^3}{216} + \mathcal{O}\left(\bar{u}_0^4\right) . \end{aligned} \tag{43}$$

The ground-state energy is then given by

$$\begin{aligned}E_{\rm gs}(\bar{u}_0) &= \Gamma_{\rm Hartree}[\rho_{\rm gs,Hartree}] \\ &= \frac{\bar{u}_0}{24} - \frac{\bar{u}_0^2}{144} + \frac{5\bar{u}_0^3}{2592} + \mathcal{O}\left(\bar{u}_0^4\right) . \end{aligned} \tag{44}$$

Clearly, the Hartree approximation does not reproduce the exact results, even in the small-coupling limit. In fact, it significantly underestimates the exact results for $E_{\rm gs}$ and overestimates those for the ground-state $\rho_{\rm gs}$.

In Fig. 2 we show our results for $E_{\rm gs}$ and $\rho_{\rm gs}$. The comparison of the exact results with the results from a small-coupling expansion at leading and next-to-leading order shows that the latter are only meaningful for $\bar{u}_0 \lesssim 0.2$. The results from the Hartree approximation are not in agreement with the exact results, neither at small coupling nor at strong coupling. For $\bar{u}_0 = 1$, for example, the relative error of the Hartree expansion amounts to about 57%.

For illustration purposes, we now compute $E_{\rm gs}$ and $\rho_{\rm gs}$ with our flow equation (11). In the present case, it assumes a simple form:

$$\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{24}\bar{u}_0\omega^4\left[\rho^2 + \left(\frac{\delta\Gamma_\lambda[\rho]}{\delta\rho\delta\rho}\right)^{-1}\right] . \tag{45}$$

In order to solve this equation, we expand $\Gamma[\rho]$ about the current ground-state $\rho_{{\rm gs},\lambda}$, see also Eq. (14):

$$\Gamma_\lambda[\rho] = \Gamma_\lambda[\rho_{{\rm gs},\lambda}] + \sum_{n=2}^{N_{\rm max}} \frac{1}{n!}\Gamma_\lambda^{(n)}[\rho_{{\rm gs},\lambda}](\rho - \rho_{{\rm gs},\lambda})^n , \tag{46}$$

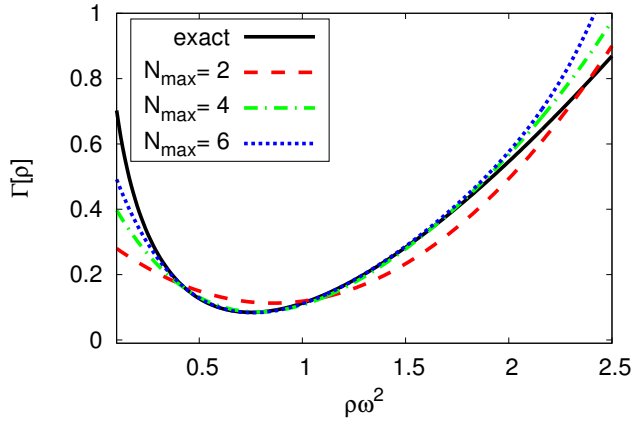

Figure 3. Effective action $\Gamma[\rho] \equiv \Gamma_{\lambda=1}[\rho]$ of the zero-dimensional toy model as obtained from our RG approach for various values of $N_{\max}$ for fixed $\bar{u}_0 = 1$. Again, we have normalized the effective action such that $\Gamma_{\lambda=1}[\rho_{\rm gs}] = 0$ for $\bar{u}_0 = 0$.

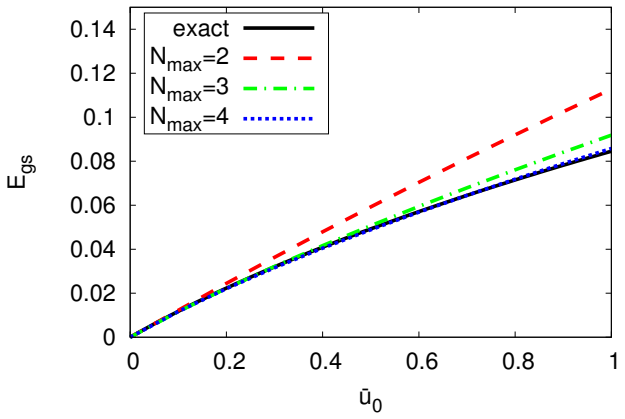

Figure 4. $E_{\rm gs}$ as a function of $\bar{u}_0$ as obtained from our RG study. Note that our results for $N_{\max} = 4$ are already almost indistinguishable from the exact values for $E_{\rm gs}$ on the scale of the plot.

where $N_{\max}$ denotes the order of the truncation. Note that $\partial_\lambda \Gamma^{(1)}_\lambda[\rho_{{\rm gs},\lambda}] \equiv 0$ and $\Gamma^{(1)}_{\lambda=0}[\rho_{{\rm gs},\lambda}] \equiv 0$ by definition. Plugging this expansion into the flow equation (45) then yields a tower of flow equations for $E_{{\rm gs},\lambda} = \Gamma_\lambda[\rho_{{\rm gs},\lambda}]$, $\rho_{{\rm gs},\lambda}$, and the n-point functions $\Gamma^{(n)}_\lambda[\rho_{{\rm gs},\lambda}]$. The initial conditions for these flow equations can be extracted by expanding $\Gamma_{\bar{u}_0=0}[\rho]$ about its ground state $\rho_{\rm gs}$.

For $N_{\max} = 2$, for example, we find the following set of coupled ordinary first-order differential equations:

$$\partial_\lambda E_{{\rm gs},\lambda} = \frac{1}{24}\bar{u}_0\omega^4 \left[\rho_{\rm gs}^2 + \left(\Gamma^{(2)}_\lambda[\rho_{{\rm gs},\lambda}]\right)^{-1}\right], \quad (47)$$

$$\partial_\lambda \rho_{{\rm gs},\lambda} = -\frac{1}{12}\bar{u}_0\omega^4\rho_{\rm gs}\left(\Gamma^{(2)}_\lambda[\rho_{{\rm gs},\lambda}]\right)^{-1}, \quad (48)$$

$$\partial_\lambda \Gamma^{(2)}_\lambda[\rho_{{\rm gs},\lambda}] = \frac{1}{12}\bar{u}_0\omega^4. \quad (49)$$

Note that $N_{\max} = 2$ is sufficient to exactly reproduce the perturbative results for the ground-state energy $E_{\rm gs}$ at leading order. In order to correctly reproduce the leading order of the perturbative expansion of the ground state $\rho_{\rm gs}$ and the n-point functions of higher order, we need to increase the truncation order beyond $N_{\max} = 2$. From our general discussion above, it follows that $N_{\max} = 4$ is sufficient to correctly reproduce the perturbative series of $\rho_{\rm gs}$ and $\Gamma^{(2)}_\lambda[\rho_{{\rm gs},\lambda}]$ at leading order. Moreover, we also recover the correct results for $E_{\rm gs}$ at next-to-leading order with $N_{\max} = 4$.

We would like to add that the set of flow equations for $N_{\max} = 2$ can be solved analytically. We refrain from giving the explicit result here. We only state that the ground-state energy behaves as

$$E_{\rm gs}(\bar{u}_0) \sim \ln \bar{u}_0 . \quad (50)$$

This is in accordance with the asymptotic behavior of the exact result, only that the coefficient of this term is not reproduced correctly for $N_{\max} = 2$.

In Fig. 3, we present our results for $\Gamma[\rho] \equiv \Gamma_{\lambda=1}[\rho]$ as a function of ρ for various values of $N_{\max}$ for fixed $\bar{u}_0 = 1$. Note that the radius of convergence of our expansion (46) about the ground state is finite. In fact, we find $r_\rho/\omega^2 = 1$ for the (dimensionless) radius of convergence in the case $\bar{u}_0 = 0$. Our numerical results for finite $\bar{u}_0$ are in accordance with this result. In fact, we do not observe a convergent behavior around $\rho\omega^2 \approx 2$ for increasing $N_{\max}$. On the other hand, our results for $\Gamma[\rho]$ nicely approach the exact results for $|\rho - \rho_{\rm gs}|\omega^2 \lesssim 1$ when $N_{\max}$ is increased. In order to compute $\Gamma[\rho]$ for $\rho\omega^2 > 2$, we could employ Taylor expansions around various different points with overlapping regions of convergence. This would be of importance, for example, when we expect that $\Gamma[\rho]$ develops various minima.

In Fig. 4, we present our RG results for $E_{\rm gs}$ as a function of $\bar{u}_0$ for various values for $N_{\max}$. We find that our results for $N_{\max} = 4$ are already in very good agreement with the exact results for $\bar{u}_0 \lesssim 1$ and that we approach the exact results from above for increasing $N_{\max}$. For large values of the coupling $\bar{u}_0$, we observe that we need to go to higher truncation orders in order to reproduce the exact results. Assuming that we do not know the exact solution for a given value of $\bar{u}_0$, these findings imply that we have to compute $E_{\rm gs}$ as a function of $N_{\max}$ and check numerically the convergence of this function. This is illustrated for $\bar{u}_0 = 1$ in Fig. 5. The solid (blue) line shows the result from a fit of the RG data for $N_{\max} = 2, 3, 4, 5, 6$ to the (empirical) three-parameter ansatz

$$E^{\rm RG}_{\rm gs}(N_{\max}) = E^{\rm fit}_{\rm gs} + \alpha_1 {\rm e}^{-\alpha_2 N_{\max}} . \quad (51)$$

Here, $E^{\rm fit}_{\rm gs}$, α_1, and α_2 are the three fit parameters. We obtain $E^{\rm fit}_{\rm gs} \approx 0.0833$ which is about 2% smaller than the exact result $E_{\rm gs} \approx 0.0846$.

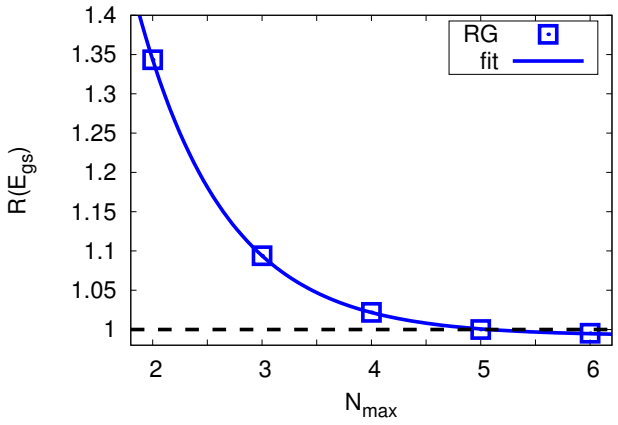

Figure 5. $R(E_{\rm gs}) = E_{\rm gs}^{\rm RG}/E_{\rm gs}^{\rm exact}$ as a function of $N_{\rm max}$ for $\bar{u}_0 = 1$. The solid (blue) line represents a fit of the RG data to the (empirical) ansatz (51), see main text for details.

B. Quantum Anharmonic Oscillator: One-dimensional Toy Model

Up to this point, we have only discussed a zero-dimensional model which essentially boils down to ordinary calculus. Let us now discuss a simple one-dimensional field-theoretical toy model described by the following classical action:

$$S = \frac{1}{2}\int_0^\beta d\tau\, \psi(\tau)\left[-\partial_\tau^2 + \omega^2\right]\psi(\tau) + \frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau' \psi(\tau)\psi(\tau')U(\tau-\tau')\psi(\tau')\psi(\tau)\,, \quad (52)$$

where $\psi(\tau)$ is a real-valued field and

$$U(\tau-\tau') = \frac{1}{12}u_0\delta(\tau-\tau')\,. \quad (53)$$

From a quantum mechanical point of view, this classical action describes nothing but the quantum anharmonic oscillator.[11] Note that $\psi(\tau)$ can be associated with a time-dependent coordinate. We have chosen the normalization factor of the interaction potential U such that it corresponds to the standard choice for this model, see, e. g., Ref. [50].

Much is known about this model. In fact, it is straightforward to diagonalize the Hamilton operator of this model numerically without any approximation, see, e. g., Ref. [51]. Thus, we have again an exact solution at hand which allows us to benchmark our RG results. We would like to add that this model has already been employed to benchmark other RG approaches, such as the 1PI RG approach [52, 53] and also 2PI approaches [54]. The large-coupling limit of this model has been studied using so-called large-N techniques, see, e. g., Ref. [50]. In the latter approach, it is straightforward to show that the ground-state energy scales as

$$E_{\rm gs} \sim \omega \bar{u}_0^{\frac{1}{3}} \quad (54)$$

for $\bar{u}_0 \gg 1$. Here, $\bar{u}_0$ is the dimensionless coupling constant which is defined as[12]

$$\bar{u}_0 = \frac{u_0}{\omega^3}\,. \quad (55)$$

In the following we use our 2PPI RG approach (DFT-RG approach) to study the ground-state properties of this model. To this end, it is convenient to expand the ground-state $\rho_{{\rm gs},\lambda}(\tau)$ and the n-point function $\Gamma_\lambda^{(n)}[\rho_{{\rm gs},\lambda}]$ in a Fourier series. For the ground-state, we choose

$$\rho_{{\rm gs},\lambda}(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty}\rho_\lambda^{(n)} e^{i\omega_n\tau}\,, \quad (56)$$

where $\omega_n = 2\pi n/\beta$. Note that the fields $\psi(\tau)$ are real-valued fields and therefore obey periodic boundary conditions in the imaginary-time direction.

Rather than working with the two-point function $\Gamma_\lambda^{(2)}$, we shall use the propagator $G_\lambda(\tau,\tau')$ from now on. The latter is defined as the inverse of the two-point function:

$$\int_0^\beta d\tau'' G_\lambda(\tau,\tau'')\left[\Gamma_\lambda^{(2)}[\rho_{{\rm gs},\lambda}](\tau'',\tau')\right] = \delta(\tau-\tau')\,. \quad (57)$$

Note that G_λ should not be confused with a single-particle propagator. However, both propagators are related in simple terms, see our detailed discussion in Appendix A. The propagator can again be expanded in a Fourier series:

$$G_\lambda(\tau,\tau') = \frac{1}{\beta}\sum_{m=-\infty}^{\infty}\frac{1}{\beta}\sum_{n=-\infty}^{\infty} G_\lambda^{(m,n)} e^{i\omega_m\tau} e^{-i\omega_n\tau'}\,. \quad (58)$$

The matrix $G_\lambda^{(m,n)}$ is diagonal, i. e.

$$G_\lambda^{(m,n)} = \beta G_\lambda^{(m)}\delta_{m,n}\,. \quad (59)$$

Higher n-point functions can be expanded accordingly:

$$\Gamma_\lambda^{(n)}[\rho_{{\rm gs},\lambda}](\tau_1,\ldots,\tau_n) = \frac{1}{\beta^n}\sum_{m_1,\ldots,m_n=-\infty}^{\infty}\left(\Gamma_\lambda^{(n)}\right)^{(m_1,\ldots,m_n)} e^{i\sum_{l=1}^n \omega_{m_l}\tau_l}\,. \quad (60)$$

In order to derive the flow equations for the Fourier coefficients, we again employ our vertex expansion, see Eq. (14). Plugging the latter into the general flow equation (11), we eventually obtain the flow equations for the Fourier coefficients. The initial conditions for these RG equations are determined by the non-interacting problem ($\bar{u}_0 = 0$), see Appendix A.

[11] From a field-theoretical point of view, it corresponds to a so-called ϕ^4-theory in one dimension.

[12] Note that the dimension of the coupling in units of ω differs from the one discussed in Eq. (23). This can essentially be traced back to the fact that the time derivative appears quadratically in the action (52) of our present model rather than linearly.

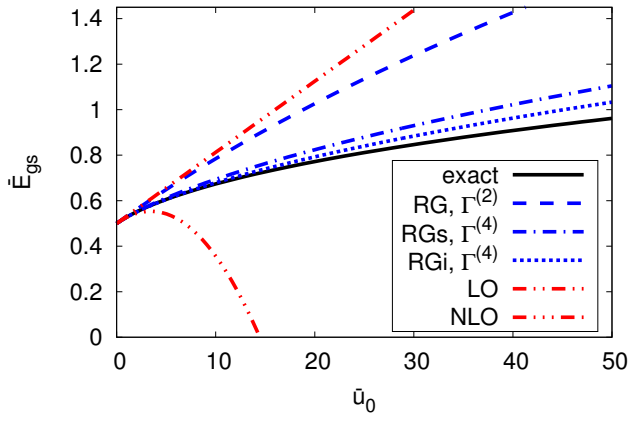

Figure 6. Comparison of the ground-state energy $E_{\rm gs}$ as a function of $\bar{u}_0$ as obtained from various different approaches. The RG results are compared with the exact results and the perturbative results at leading order (LO) and next-to-leading order (NLO). The analytic solution (68) for the leading-order RG approximation (RG, $\Gamma^{(2)}$) overestimates significantly the ground-state energy. For details on the RG approximations of higher order (RGs, $\Gamma^{(4)}$; RGi, $\Gamma^{(4)}$), we refer the reader to the main text .

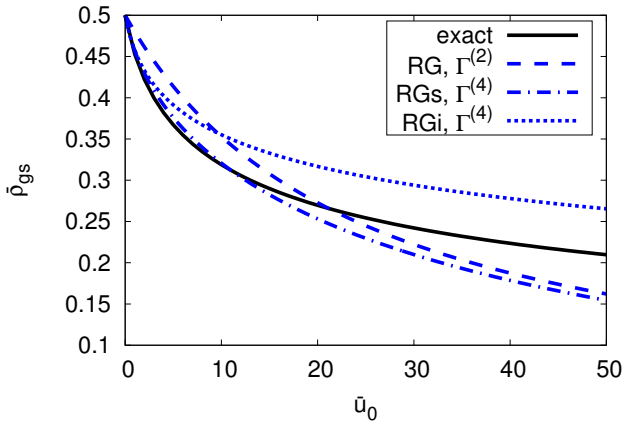

Figure 7. Comparison of the ground-state $\rho_{\rm gs}$ as a function of $\bar{u}_0$ as obtained from various different approaches. The analytic solution (72) for the leading-order RG approximation (RG, $\Gamma^{(2)}$) is not in accordance with the exact results, neither in the small coupling-limit nor for large values of the coupling, see main text for details on the higher-order RG approximations (RGs, $\Gamma^{(4)}$; RGi, $\Gamma^{(4)}$).

1. *Leading-order approximation*

Let us begin with a discussion of the lowest non-trivial approximation which is given by dropping $\Gamma^{(n)}_\lambda[\rho_{{\rm gs},\lambda}]$ as well as their RG flows for $n \geq 3$, i. e. we consider the case $N_{\rm max} = 2$. For the ground-state energy $E_{{\rm gs},\lambda}$, we then find

$$\partial_\lambda \bar{E}_{{\rm gs},\lambda} = \frac{\bar{u}_0}{24}\left[\left(\frac{1}{\bar{\beta}}\bar{\rho}^{(0)}_\lambda\right)^2 + \frac{1}{\bar{\beta}}\sum_{m=-\infty}^{\infty}\bar{G}^{(m)}_\lambda\right] . \quad (61)$$

Here, we have introduced the following dimensionless quantities:

$$\bar{E}_{{\rm gs},\lambda} = \omega^{-1}E_{{\rm gs},\lambda} , \quad (62)$$
$$\bar{\beta} = \beta\omega , \quad (63)$$
$$\bar{\rho}^{(m)}_\lambda = \omega^2\rho^{(m)}_\lambda , \quad (64)$$
$$\bar{G}^{(m)}_\lambda = \omega^3 G^{(m)}_\lambda . \quad (65)$$

In terms of these quantities, the flow equations for the Fourier coefficients associated with the ground state $\rho_{\rm gs}$ read

$$\partial_\lambda \bar{\rho}^{(m)}_\lambda = -\frac{1}{12}\bar{u}_0\bar{\rho}^{(m)}_\lambda\bar{G}^{(-m)}_\lambda . \quad (66)$$

Finally, the RG flow of the propagator is determined by the following set of equations:

$$\partial_\lambda \bar{G}^{(m)}_\lambda = -\frac{1}{12}\bar{u}_0\left(\bar{G}^{(m)}_\lambda\right)^2 . \quad (67)$$

Clearly, Eqs. (61), (66) and (67) represent an infinite set of flow equations. For the present leading-order approximation, we can still solve this set analytically. We find

$$\bar{E}_{{\rm gs},\lambda} = -\frac{1}{2} + \frac{\bar{u}_0\lambda}{4(24+\bar{u}_0\lambda)} + \sqrt{1+\frac{\bar{u}_0}{24}\lambda} . \quad (68)$$

The first two terms essentially represent the Hartree term whereas the last term originates from the third term on the right-hand side of Eq. (11). As it should be, this expression reduces to $\bar{E}_{{\rm gs},\lambda=0} = \frac{1}{2}$ at the non-interacting starting point of the flow ($\lambda = 0$). For small $\bar{u}_0$, we can expand the result for the ground-state energy and obtain

$$\bar{E}_{{\rm gs},\lambda=1} = \frac{1}{2} + \frac{1}{32}\bar{u}_0 - \frac{1}{1536}\bar{u}_0^2 + \mathcal{O}(\bar{u}_0^3) , \quad (69)$$

which needs to be compared to the exact perturbative results [50]:

$$\bar{E}^{\rm exact}_{\rm gs} = \frac{1}{2} + \frac{1}{32}\bar{u}_0 - \frac{7}{1536}\bar{u}_0^2 + \mathcal{O}(\bar{u}_0^3) . \quad (70)$$

Thus, we reproduce the perturbative result at leading order within the present approximation but not the coefficient of the second-order correction. Moreover, it follows from Eq. (68) that $\bar{E}_{\rm gs} \equiv \bar{E}_{{\rm gs},\lambda=1}$ scales as

$$\bar{E}_{\rm gs} \sim \sqrt{\bar{u}_0} \quad (71)$$

for $\bar{u}_0 \gg 1$. Apparently, this does not agree with the result from the large-N approximation, see Eq. (54). The scaling behavior of the latter has also been confirmed for the present model by solving the Schrödinger equation numerically, see, e. g., Ref. [51]. Note that the Hartree approximation renders $E_{\rm gs}$ independent of $\bar{u}_0$ in the large coupling limit.

In Fig. 6, we show our results for the ground-state energy as a function of the dimensionless coupling $\bar{u}_0$.

For comparison, we also show the exact results [51] and the perturbative results at leading and next-to-leading order. Our RG results for the ground-state energy from the leading-order approximation is in agreement with the leading-order perturbative result at small coupling but overestimates significantly the exact results for large values of $\bar{u}_0$. Thus, the present approximation is insufficient and we need to take into account n-point functions of higher order, see our discussion below.

For completeness, we also discuss the behavior of the ground-state as obtained from the present approximation. First, we note that $\bar{\rho}_\lambda^{(n)} = 0$ for $\lambda = 0$ and $n \neq 0$, see also Appendix A. For $n = 0$, we have $\bar{\rho}_{\lambda=0}^{(0)} \to \bar{\beta}/2$ for $\bar{\beta} \to \infty$. This implies that $\partial_\lambda \rho_\lambda^{(n)} = 0$ for $n \neq 0$. Thus, only the zero mode $\bar{\rho}_\lambda^{(0)}$ contributes to the flow of $\rho_{\mathrm{gs},\lambda}$:

$$\rho_{\mathrm{gs},\lambda}(\tau) \overset{\bar{\beta}\to\infty}{\longrightarrow} \frac{1}{2\omega}\frac{1}{1+\lambda\frac{\bar{u}_0}{24}}\,. \tag{72}$$

Note that $\rho_{\mathrm{gs},\lambda}(\tau)$ does not depend on the imaginary time τ.

Our results for $\rho_{\mathrm{gs},\lambda}(\tau)$ are shown in Fig. 7. Since the three-point function $\Gamma_\lambda^{(3)}$ contributes to the flow of the ground state ρ_{gs} already at leading order, we do not even recover the leading-order perturbative result with our present truncation. For example, this becomes apparent from the comparison with the exact result in the small coupling-limit. The same line of arguments holds for the propagator. In fact, not only the three-point function $\Gamma_\lambda^{(3)}$ contributes to the flow of the propagator but also the four-point function $\Gamma_\lambda^{(4)}$.

2. Higher-order approximations

Let us now discuss the role of n-point functions of higher order. As discussed in Sect. II, it can be shown that the RG flow of the n-point function depends on the flow of the $n+1$ and $n+2$-point function. Since the ground-state is associated with the one-point function,[13] this means that the two- and the three-point function govern the RG flow of ρ_{gs}. In fact, the most general form of the flow equation for the ground state ρ_{gs} of our present model with a constant background potential is given by

$$\partial_\lambda \bar{\rho}_\lambda^{(l)} = -\frac{\bar{u}_0}{24}\Bigg[2\bar{\rho}_\lambda^{(l)}\bar{G}_\lambda^{(-l)} + \frac{\delta_{l,0}}{\bar{\beta}}\sum_{k=-\infty}^{\infty}\bar{G}_\lambda^{(l)}\left(\bar{G}_\lambda^{(k)}\right)^2\left(\bar{\Gamma}_\lambda^{(3)}\right)^{(k,-k,l)}\Bigg]. \tag{73}$$

Since $\bar{\rho}_\lambda^{(n)} = 0$ for $\lambda = 0$ and $n \neq 0$, only the flow of the zero mode $\bar{\rho}_\lambda^{(0)}$ is vanishing and therefore only $\bar{\rho}_\lambda^{(0)}$ assumes a finite value. From this observation, it follows immediately that the ground state ρ_{gs} does not depend on the imaginary time. This remains true even for $d+1$-dimensional field theories, provided that we consider an interaction potential of the form $U \sim \delta(\tau - \tau')$. In any case, from the general flow equation for the ground state it is apparent that the three-point function contributes to the ground-state at leading order in a perturbative expansion.

Let us now turn to the most general flow equation for the propagator (inverse two-point function). This flow equation depends on the RG flows of the three- and four-point function and can be written as follows

$$\begin{aligned}\partial_\lambda \bar{G}_\lambda^{(m)} = -\frac{\bar{u}_0}{12}\Bigg[&\left(\bar{G}_\lambda^{(m)}\right)^2 - \frac{1}{\bar{\beta}^2}\sum_{l=-\infty}^{\infty}\bar{\rho}_\lambda^{(l)}\bar{G}_\lambda^{(-l)}\left(\bar{G}_\lambda^{(m)}\right)^2\left(\bar{\Gamma}_\lambda^{(3)}\right)^{(-l,m,-m)} - \frac{1}{6}\frac{1}{\bar{\beta}^2}\sum_{k=-\infty}^{\infty}\left(\bar{G}_\lambda^{(m)}\right)^2\left(\bar{G}_\lambda^{(k)}\right)^2\left(\bar{\Gamma}_\lambda^{(4)}\right)^{(k,m,-k,-m)} \\ &+\frac{1}{2}\frac{1}{\bar{\beta}^3}\sum_{l=-\infty}^{\infty}\sum_{k=-\infty}^{\infty}\bar{G}_\lambda^{(-l)}\left(\bar{G}_\lambda^{(m)}\right)^2\left(\bar{G}_\lambda^{(k)}\right)^2\left(\bar{\Gamma}_\lambda^{(3)}\right)^{(k,-k,l)}\left(\bar{\Gamma}_\lambda^{(3)}\right)^{(-l,m,-m)} \\ &+\frac{1}{\bar{\beta}^3}\sum_{l=-\infty}^{\infty}\sum_{k=-\infty}^{\infty}\left(\bar{G}_\lambda^{(m)}\right)^2\left(\bar{G}_\lambda^{(k)}\right)^2\bar{G}_\lambda^{(m+k)}\left(\bar{\Gamma}_\lambda^{(3)}\right)^{(k,m,l)}\left(\bar{\Gamma}_\lambda^{(3)}\right)^{(-l,-m,-k)} \\ &-\frac{1}{3}\frac{1}{\bar{\beta}^2}\sum_{k=-\infty}^{\infty}\left(\bar{G}_\lambda^{(m)}\right)^2\left(\bar{G}_\lambda^{(k)}\right)^2\left(\bar{\Gamma}_\lambda^{(4)}\right)^{(k,-k,m,-m)}\Bigg].\end{aligned} \tag{74}$$

Since the right-hand side is proportional to the coupling $\bar{u}_0$, we conclude that we need to include the three- and four-point function in our study in order to recover the correct perturbative result at leading order. The inclusion of these two correlation functions in the flow of the propagator then also guarantees that the results for the ground-state energy agree with perturbation theory up to second order in the small-coupling limit, see our

[13] The flow equation for the ground state follows from the stationary condition $(\delta\Gamma/\delta\rho)|_{\mathrm{gs}} = 0$.

general discussion in Sect. II C.

For simplicity, we do not include the full flow of the three- and four-point function in our numerical studies in the following. We rather use a 'static' approximation for these correlation functions, i. e. we set their flow equations to zero, $\partial_\lambda \Gamma_\lambda^{(3)} = \partial_\lambda \Gamma_\lambda^{(4)} = 0$, but we do not set the functions themselves to zero. Recall that $\Gamma_\lambda^{(3)}$ and $\Gamma_\lambda^{(4)}$ are not identical to zero at the initial point of the RG flow ($\lambda = 0$), see also Appendix A. Moreover, we set the n-point correlation functions with $n > 4$ to zero as well as their flows.

Using this approximation, we recover the correct leading-order behavior of the propagator and the ground-state $\rho_{\rm gs}$ in the small-coupling limit. Moreover, the ground-state energy is correct up to second order in this limit, as we have checked analytically.

In order to go beyond the perturbative small-coupling limit, we have to solve the set of flow equations (61), (73), and (74) numerically. To this end, we have to truncate the sum over the Fourier coefficients, i. e. we only take into account the coefficients up to a certain value $N_{\rm max}^{\rm Fourier}$. Here and in our subsequent study including an RG improvement, we choose $N_{\rm max}^{\rm Fourier} = 100$ and $(\bar\beta)^{-1} = T/\omega = 0.1$ for the dimensionless temperature. We have also applied this choice to the lowest-order RG approximation and compared the results to the corresponding analytic solution. For $\bar u_0 \lesssim 50$, we have found that our numerical results for $E_{\rm gs}$ and $\rho_{\rm gs}$ deviate from the analytic ones by about 1% or less.[14]

In Fig. 6, we present our numerical results for the ground-state energy obtained with this approximation (labelled as 'RGs, $\Gamma^{(4)}$'). The ground-state is shown in Fig. 7. We observe that the ground-state energy is now in reasonable agreement with the exact result. To be more specific, we find that the ground-state energy is less than 5% larger than the exact value at $\bar u_0 = 10$. For $\bar u_0 = 20$, however, we still have an error of about 10%. In any case, the inclusion of $\Gamma_\lambda^{(3)}$ and $\Gamma_\lambda^{(4)}$ in our static approximation already yields a drastic improvement of our results obtained with the leading-order approximation. With respect to the ground-state, we now find good agreement between our results and the exact results for $\bar u_0 \lesssim 2$. For larger values of the coupling, we observe that our results deviate significantly from the exact results. In fact, also the asymptotic functional form of $\rho_{\rm gs}$ turns out to be incorrect.

3. RG improvement

Let us now discuss how our RG flows can be improved. To this end, we consider the approximation which we have just discussed. The results for $E_{\rm gs}$ from this approximation are already in reasonable agreement with the exact result for $\bar u_0 \lesssim 20$. For larger values of the coupling, this approximation suffers from the fact that we have only included $\Gamma_\lambda^{(3)}$ and $\Gamma_\lambda^{(4)}$ 'statically', i. e. we have dropped the flow of these correlation functions. Now we would like to improve our set of flow equations without explicitly taking into account the RG flow equations for $\Gamma_\lambda^{(3)}$ and $\Gamma_\lambda^{(4)}$.

First, we note that the oscillator frequency ω effectively changes when the interaction is turned on. To be more specific, ω effectively increases with increasing $\bar u_0$ due to quantum corrections. This becomes apparent when we look at the $\bar u_0$-dependence of the ground state $\rho_{\rm gs}$. At $\lambda = 0$ (non-interacting limit), we have

$$\rho_{{\rm gs},\lambda=0} = \frac{1}{2\omega} \tag{75}$$

for $\beta \to \infty$. Now recall that for increasing λ and/or $\bar u_0$, the value for the ground state $\rho_{{\rm gs},\lambda}$ decreases, see also Eq. (72). Thus, a change of the ground state can therefore be viewed as an effective change of the oscillator frequency. In this spirit, we define an effective λ-dependent oscillator frequency $\omega_\lambda^{\rm eff.}$:

$$\omega_\lambda^{\rm eff.} := \frac{1}{2}\left(\rho_{{\rm gs},\lambda}\right)^{-1} . \tag{76}$$

In terms of the only non-vanishing Fourier coefficient of the ground-state, this can be written as follows:

$$\bar\omega_\lambda^{\rm eff.} = \frac{\omega_\lambda^{\rm eff.}}{\omega} = \frac{\bar\beta}{2}\left(\bar\rho_{{\rm gs},\lambda}^{(0)}\right)^{-1} . \tag{77}$$

With this effective oscillatory frequency at hand, we can improve our set of RG equations for the ground-state and the propagator. To this end we exploit the fact that $\Gamma_{\lambda=0}^{(3)}$ and $\Gamma_{\lambda=0}^{(4)}$ depend on the oscillatory frequency ω. We now replace ω with the effective λ-dependent (flowing) oscillatory frequency $\omega_\lambda^{\rm eff.}$. This can be viewed as an inclusion of the three- and four-point function associated with a harmonic oscillator with frequency $\omega_\lambda^{\rm eff.}$. Since $\omega_\lambda^{\rm eff.}$ is a non-trivial function of $\bar u_0$, this improvement allows us to include corrections of higher order in a simple manner.

We would like to add that the change of $\Gamma_\lambda^{(3)}$ and $\Gamma_\lambda^{(4)}$ under a variation of λ is in principle governed by flow equations which we have not taken into account in the present study. In this respect, our improvement can also be considered as a way to estimate the impact of neglected n-point functions of higher order. Recall that the flow of a given n-point function depends on the $n+1$- and $n+2$-point function. This implies that we have in general to deal with an infinite tower of flow equations. Even if we had included the full flow equations for the three- and four-point function, we would still require information about the five- and six-point function. Since this tower of equations needs to be truncated at some order, it is always desirable to estimate to some extent the effect of the neglected n-point functions. Our proposed

[14] For increasing $\bar u_0$, we have to increase $N_{\rm max}^{\rm Fourier}$ in order to reproduce the analytic results.

RG improvement represents one possibility for such an estimate.

Let us now turn to the (numerical) results from our improved RG flows. From the construction of these flows, it is clear that we still recover the correct perturbative result for the ground-state energy up to second order. To see this, we note that $\omega_\lambda^{\text{eff.}}$ can be expanded in a power series of $\bar{u}_0$. Our improved three- and four-point functions therefore also have a well-defined perturbative expansion:

$$\Gamma^{(n)}_{\lambda=0}\Big|_{\omega=\omega_\lambda^{\text{eff.}}} - \Gamma^{(n)}_{\lambda=0}\Big|_{\omega} = \left(\frac{\partial\omega_\lambda^{\text{eff.}}}{\partial\bar{u}_0}\right)\left(\frac{\partial\Gamma^{(n)}_{\lambda=0}}{\partial\omega}\right)_{\omega=\omega_\lambda^{\text{eff.}}} \bar{u}_0 + \mathcal{O}(\bar{u}_0^2)\,. \quad (78)$$

From this expression, it is apparent that the improvement only affects the third order of the perturbative expansion of the RG flow equation for the ground-state energy. For the ground state ρ_{gs}, the second order already receives contributions from our RG improvement. The latter statement also holds for the propagator. In Fig. 6 we show our results for the ground-state energy obtained with this RG improvement (labelled as 'RGi, $\Gamma^{(4)}$'). The results for the ground-state are given in Fig. 7. We observe that the improvement brings our RG results for E_{gs} and ρ_{gs} closer to the corresponding exact values. In fact, we find that the ground-state energy now deviates less than 2% from the exact value at $\bar{u}_0 = 10$. For $\bar{u}_0 = 20$, we have an error of about 5%. We would like to add that our RG results for the ground-state energy approach the exact results from above when we include n-point functions of higher order. Comparing our results for ρ_{gs} with the exact values, it even appears that our results are now consistent with the asymptotic functional form of ρ_{gs} for large values of the coupling.

IV. CONCLUSIONS AND OUTLOOK

We have discussed an RG approach to DFT and analyzed its properties on very general grounds, including its relation to perturbation theory and the computation of excited states. A special feature of this approach is that it does not rely on a (global) parameterization of the density functional. The RG flow rather starts at a well-defined analytically accessible starting point. By gradually increasing the *microscopic* interactions, the underlying RG flow equation then allows us to follow the ground-state of the theory.

The presented RG approach eventually aims at a study of ground-state properties of non-relativistic self-bound fermionic systems, such as (heavy) nuclei, from microscopic interactions. In the present work, however, we have restricted ourselves to studies of two simple toy models which nevertheless helped us to already test and benchmark our approach in a simple but meaningful manner for future studies. From a theoretical point of view, these two models correspond to a zero and one-dimensional field theory. In the present paper, the latter was nothing but the quantum anharmonic oscillator.

Our toy model studies allowed us to illustrate how our RG approach works in general and how ground-state properties of physical systems can be computed with this novel tool. An important feature of our approach is that the so-called 2PPI effective action (corresponding to the energy density functional) can be computed systematically from the underlying microscopic interactions by means of a vertex expansion. With respect to nuclear physics, this implies that our DFT-RG approach opens up a new direction to compute the energy density functional from, e. g., chiral EFT interactions. Apart from the explicit (quantitative) computation of energy functionals and ground-state properties, the presented RG approach can be viewed as a tool to gain deeper insights into the general structure of density functionals. For example, we have demonstrated how a connection between the energy density functional and perturbation theory can be established in a simple and systematic fashion.

For our toy models, we have found that the RG results for, e. g., the ground-state energy are in reasonable agreement with the exact results over a wide range of values for the (microscopic) coupling constant, even if we only take into account correlation functions up to the four-point function. By comparing our results with the exact results, we have also demonstrated that the quality of the RG results can be systematically improved by taking into account n-point functions of higher order.

The present work should be considered as a starting point for various studies. For example, we have already mentioned the relation of the present DFT-RG approach to the 1PI RG approach [41]. It would also be interesting to better understand how it relates to other RG approaches widely used to study the nuclear many-body problem [55–58]. Apart from these more field-theoretically motivated formal studies, another natural next step is now to study ground-state properties of so-called Alexandrou-Negele nuclei [59]. These are self-bound systems in one space and one time dimension, consisting of N spinless fermions interacting via a specific choice for a long-range attractive and short-range repulsive potential U. In this case, the initial condition at $\lambda = 0$ corresponds to a simple harmonic oscillator potential in which the N lowest lying levels are filled. By solving the RG flow equation (11), we then gradually remove the background potential V and turn on the two-body interaction potential U. The RG results for these systems can be benchmarked against those from *ab-initio* MC calculations [59] and studies with the so-called similarity RG approach [56]. The present work will help us to set up these studies of one-dimensional nuclei [35]. The latter will then help us to further develop and establish our novel DFT-RG approach and may pave the way for the computation of ground-state properties of realistic nuclei from microscopic interactions in a novel alternative way.

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Appendix A: Initial Conditions

In this appendix we discuss the computation of the initial conditions for our one-dimensional toy model. In the spirit of our vertex expansion, we expand the effective action about the ground state $\rho_{\rm gs}$, see Eq. (14). Along these lines we also expand the source J about $\rho_{\rm gs}$:

$$J[\rho] = \int_{\tau'} j_1(\tau,\tau')[\rho(\tau')-\rho_{\rm gs}(\tau')] + \frac{1}{2}\int_{\tau'}\int_{\tau''} j_2(\tau,\tau',\tau'')[\rho(\tau')-\rho_{\rm gs}(\tau')]\times \times[\rho(\tau'')-\rho_{\rm gs}(\tau'')] + \dots . \quad \text{(A1)}$$

Recall that J is a function of τ but also a functional of ρ. At the physical ground state $\rho_{\rm gs}$, we have $J[\rho=\rho_{\rm gs}]=0$. Using Eqs. (6) and (14), we then find

$$j_1 = \Gamma_0^{(2)}, \qquad j_2 = \Gamma_0^{(3)}, \qquad \dots . \quad \text{(A2)}$$

Here and in the following we use the index '0' (corresponding to $\lambda = 0$) to indicate that we are only discussing the non-interacting limit which determines the initial conditions for our RG flow equations.

For a non-interacting theory, the functional W_0 is given by

$$W_0[J] = -\frac{1}{2}\mathrm{Tr}\ln\left(\Delta_0^{-1}-2\tilde{J}\right) = -\frac{1}{2}\mathrm{Tr}\ln\Delta_0^{-1}+\frac{1}{2}\sum_{n=1}^{\infty}\frac{1}{n}\mathrm{Tr}\left[\left(2\Delta_0\cdot\tilde{J}\right)^n\right], \quad \text{(A3)}$$

where Δ_0^{-1} denotes the (conventional) propagator and $\tilde{J}$ is related to the source J:

$$\tilde{J}(\tau,\tau') = J(\tau)\delta(\tau-\tau'). \quad \text{(A4)}$$

From a comparison of Eq. (A3) with the expansion (14) of the effective action, we immediately obtain Γ_0:

$$\Gamma_0[\rho_{\rm gs}] = \frac{1}{2}\mathrm{Tr}\ln\Delta_0^{-1}. \quad \text{(A5)}$$

For the propagator (inverse density-density correlator), we find

$$G_0(\tau,\tau') = 2\Delta_0(\tau,\tau')\Delta_0(\tau',\tau), \quad \text{(A6)}$$

where

$$\Delta_0(\tau,\tau') = \frac{1}{\beta}\sum_{n=-\infty}^{\infty}\frac{1}{\omega_n^2+\omega^2}\,\mathrm{e}^{\mathrm{i}\omega_n(\tau-\tau')}. \quad \text{(A7)}$$

Note that $\Delta_0(\tau,\tau') = \Delta_0(\tau',\tau)$. Inserting Eq. (A7) into Eq. (A5) we obtain $\Gamma_0[\rho_{\rm gs}]$ for the non-interacting system:

$$\Gamma_0[\rho_{\rm gs}] = \frac{\beta\omega}{2} + \ln\left(1-e^{-\beta\omega}\right). \quad \text{(A8)}$$

From this expression, we can then extract the ground-state energy:

$$E_{\rm gs} = \lim_{\beta\to\infty}\frac{1}{\beta}\Gamma_0[\rho_{\rm gs}] = \frac{\omega}{2}. \quad \text{(A9)}$$

Next, we compute the Fourier expansion coefficients associated with the propagator G defined in Eq. (58). Using Eq. (A6), we find

$$G_0^{(n)} = \frac{2}{\omega\left(\omega_n^2+4\omega^2\right)}\coth\left(\frac{\beta\omega}{2}\right). \quad \text{(A10)}$$

These coefficients serve as initial conditions for the RG flow of the propagator in our study of the one-dimensional toy model.

Let us now turn to the ground state $\rho_{\rm gs}$ of the non-interacting theory. To this end, we consider the relation between ρ and the functional W_0:

$$\rho(\tau) = \frac{\delta W_0}{\delta J(\tau)} = \Delta_0(\tau,\tau) + 2\int_0^\beta d\tau'\Delta_0(\tau',\tau)\Delta_0(\tau,\tau')J(\tau') + \dots . \quad \text{(A11)}$$

From this expression, we deduce that

$$\rho_{\rm gs}(\tau) = \Delta_0(\tau,\tau) = \frac{1}{2\omega}\coth\left(\frac{\beta\omega}{2}\right). \quad \text{(A12)}$$

It then follows that the Fourier expansion coefficients defined in Eq. (56) are given by

$$\rho_{\rm gs}^{(n)} = \frac{\beta}{2\omega}\coth\left(\frac{\beta\omega}{2}\right)\delta_{n,0}. \quad \text{(A13)}$$

Moreover, we find

$$(\rho(\tau)-\rho_{\rm gs}(\tau)) = 2\int_0^\beta d\tau'\Delta_0(\tau',\tau)\Delta_0(\tau,\tau')J(\tau')+\dots . \quad \text{(A14)}$$

Plugging the expansion (A1) into this expression, we obtain

$$(\rho(\tau)-\rho_{\rm gs}(\tau)) = \int_0^\beta d\tau' G_0(\tau,\tau')\Big[\int_0^\beta d\tau''\, j_1(\tau',\tau'')[\rho(\tau'')-\rho_{\rm gs}(\tau'')] + \frac{1}{2}\int_0^\beta d\tau''\int_0^\beta d\tau'''\, j_2(\tau',\tau'',\tau''')[\rho(\tau'')-\rho_{\rm gs}(\tau'')][\rho(\tau''')-\rho_{\rm gs}(\tau''')]+\dots\Big]+\dots\,. \quad \text{(A15)}$$

Here, we have used Eq. (A6) and $G_0(\tau,\tau') = G_0(\tau',\tau)$. In order to determine the expansion coefficients j_n, we compare the left- and right-hand side order by order in our functional Taylor expansion in powers of $(\rho-\rho_{\rm gs})$. For the coefficient j_1, we obtain

$$\int d\tau' G_0(\tau,\tau') j_1(\tau',\tau'') = \delta(\tau-\tau'')\,. \quad \text{(A16)}$$

Thus, we have

$$j_1(\tau,\tau') = G_0^{-1}(\tau,\tau') = \Gamma_0^{(2)}(\tau,\tau')\,. \quad \text{(A17)}$$

Next, we would like to find a simple relation for $\Gamma^{(3)}$. This can be done along the lines of our derivation (A17). However, we now need to expand the right-hand side of Eq. (A14) up to second order in the source J. From a comparison of the expansion coefficients on the left- and right-hand side, we then find

$$\begin{aligned}\Gamma_0^{(3)}(\tau,\tau',\tau'') &= j_2(\tau,\tau',\tau'')\\ &= -8\int_0^\beta d\tau'''\int_0^\beta d\tau''''\int_0^\beta d\tau'''''\, G_0^{-1}(\tau,\tau''')\Delta_0(\tau''',\tau'''')G_0^{-1}(\tau'''',\tau')\Delta_0(\tau'''',\tau''''')G_0^{-1}(\tau''''',\tau'')\Delta_0(\tau''''',\tau''')\,, \end{aligned} \quad \text{(A18)}$$

where we have used Eq. (A17). The Fourier expansion coefficients of the three-point functions can be computed straightforwardly and read

$$\left(\Gamma_0^{(3)}\right)^{(k,l,m)} = -\frac{\beta\omega^2}{\left(\coth\left(\frac{1}{2}\beta\omega\right)\right)^2}\left(\omega_k^2+\omega_k\omega_l+\omega_l^2+12\omega^2\right)\delta_{k+l+m,0}\,. \quad \text{(A19)}$$

In our discussion of the one-dimensional toy model, we also used the initial condition of the four-point function. The computation of this correlation function (as well as of correlation functions of higher order) for the non-interacting theory can be done following the procedure detailed above. For the coefficients of the Fourier expansion of the four-point function we then obtain

$$\begin{aligned}\left(\Gamma_0^{(4)}\right)^{(k,l,m,n)} = \frac{3\beta\omega^3}{\left(\coth\left(\frac{1}{2}\beta\omega\right)\right)^3}\Big[&\left(\omega_{k+l}^2+\omega_{k+l}\omega_m+\omega_m^2+12\omega^2\right)\left(\omega_k^2+\omega_k\omega_l+\omega_l^2+12\omega^2\right)\left(\omega_{k+l}^2+4\omega^2\right)^{-1}\\ &+\left(\omega_l^2+\omega_l\omega_m+\omega_m^2+12\omega^2\right)\left(\omega_k^2+\omega_k\omega_{l+m}+\omega_{l+m}^2+12\omega^2\right)\left(\omega_{l+m}^2+4\omega^2\right)^{-1}\\ &-f(\omega_k,\omega_l,\omega_m,\omega)\left(\left(\omega_{k+l}^2+4\omega^2\right)\left(\omega_{l+m}^2+4\omega^2\right)\right)^{-1}\Big]\delta_{k+l+m+n,0}\,, \end{aligned} \quad \text{(A20)}$$

where

$$
\begin{aligned}
f(\omega_k,\omega_l,\omega_m,\omega) = \; & 640\omega^6 + 48\omega^4\left[3\omega_k^2 + 4\omega_l^2 + 4\omega_l\omega_m + 3\omega_m^2 + 2\omega_k(2\omega_l+\omega_m)\right] \\
& +4\omega^2\left[3\omega_k^4 + 2\omega_l^4 + 4\omega_l^3\omega_m + 10\omega_l^2\omega_m^2 + 8\omega_l\omega_m^3 + 3\omega_m^4 + 4\omega_k^3(2\omega_l+\omega_m)\right. \\
& \left.+2\omega_k(2\omega_l+\omega_m)(\omega_l^2+\omega_l\omega_m+2\omega_m^2) + 2\omega_k^2(5\omega_l^2+5\omega_l\omega_m+2\omega_m^2)\right] \\
& +\omega_l^2\omega_m^2(\omega_l+\omega_m)^2 + \omega_k\omega_l\omega_m^2(\omega_l+\omega_m)(2\omega_l+\omega_m) + \omega_k^4(\omega_l^2+\omega_l\omega_m+\omega_m^2) \\
& +\omega_k^3(2\omega_l+\omega_m)(\omega_l^2+\omega_l\omega_m+2\omega_m^2) + \omega_k^2(\omega_l^4+2\omega_l^3\omega_m+6\omega_l^2\omega_m^2+5\omega_l\omega_m^3+\omega_m^4)\,. \qquad \text{(A21)}
\end{aligned}
$$

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